# Heteroclinic travelling waves in convex FPU-type chains

Michael Herrmann\* Jens D.M. Rademacher<sup>†</sup>

November 3, 2009

#### Abstract

We consider infinite FPU-type atomic chains with general convex potentials and study the existence of monotone fronts that are heteroclinic travelling waves connecting constant asymptotic states. Iooss showed that small amplitude fronts bifurcate from convex-concave turning points of the force. In this paper we prove that fronts exist for any asymptotic states that satisfy certain constraints. For potentials whose derivative has exactly one turning point these constraints precisely mean that the front corresponds to an energy conserving supersonic shock of the 'p-system', which is the naive hyperbolic continuum limit of the chain. The proof goes via minimizing an action functional for the deviation from this discontinuous shock profile. We also discuss qualitative properties and the numerical computation of fronts.

Keywords: Fermi-Pasta-Ulam chain, heteroclinic travelling waves, conservative shocks, least action

MSC (2000): 37K60, 47J30, 70F45, 74J30

### 1 Introduction

We consider infinite chains of identical particles as plotted in Figure 1. These are nearest neighbour coupled in a convex potential  $\Phi : \mathbb{R} \to \mathbb{R}$  by Newton's equations

$$\ddot{x}_{\alpha} = \Phi'(x_{\alpha+1} - x_{\alpha}) - \Phi'(x_{\alpha} - x_{\alpha-1}),\tag{1}$$

where  $\dot{}=\frac{\mathrm{d}}{\mathrm{d}t}$  is the time derivative,  $x_{\alpha}(t)$  the atomic position,  $\alpha \in \mathbb{Z}$  the particle index.

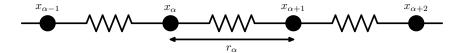


Figure 1: The atomic chain with nearest neighbour interaction.

Such chains model particles connected by springs in one dimension and serve as simplified models for crystals and solids. In their seminal paper [FPU55] Fermi, Pasta and Ulam studied such chains assuming that the interaction potential  $\Phi$  contains at most quartic terms. We consider convex  $\Phi$  with nonlinear force function  $\Phi'$  and allow for turning points, i.e., points where  $\Phi''' = 0$ , but still refer to (1) as FPU chains. In fact, the existence of fronts, which is studied in this paper, requires that  $\Phi'$  has at least one turning point, see [HR08], and this excludes, for instance, the famous Toda potential.

One focus of the research concerns solutions with coherent structures, in particular travelling waves, for which there exists a smooth profile that travels with constant speed and shape through the chain.

<sup>\*</sup>University of Oxford, Mathematical Institute, Centre for Nonlinear PDE (OxPDE), 24-29 St Giles', Oxford OX1 3LB, United Kingdom, michael.herrmann@maths.ox.ac.uk.

<sup>&</sup>lt;sup>†</sup>National Research Centre for Mathematics and Computer Science (CWI), Science Park 123, 1098 XG Amsterdam, the Netherlands, rademach@cwi.nl.

The main types of travelling waves are periodic wave trains, homoclinic solitons (or solitary waves), and heteroclinic fronts. Mathematically, rigorous existence proofs of such solutions are an important basic issue. During the last two decades a lot of research addressed the existence of solitons and wave trains: [FW94, FV99, Her05, DHM06] establish the existence of such waves by solving constrained optimisation problems, [SW97, PP00, Pan05, SZ07] apply the Mountain Path Theorem to the action integral for travelling waves, and [Ioo00] uses center manifold reduction with respect to the spatial dynamics.

In comparison, little is known rigorously for fronts. For (non-smooth and non-convex) double-well potentials composed of the same quadratic parabolas, the existence of fronts connecting oscillatory states has been recently shown in [SZ08]. Such fronts can be interpreted as phase transitions and more physical results can be found for instance in [SCC05, TV05].

In these cases the connection between fronts and shocks in the naive continuum limit of (1) was crucial. This limit is the so-called p-system formed by the hyperbolic conservation laws for mass and momentum. Shocks in the p-system come in different types given by the relation of their speed and the sound speed of the asymptotic states: shocks that are faster (slower) than these sound speeds are called supersonic (subsonic). The fronts found in [SZ08] for the quadratic double-well case correspond to subsonic shocks when taking the average of the asymptotic oscillations. It turns out that these shocks also balance the energy jump relation, and we refer to such shocks as conservative.

The connection to p-system shocks is also crucial for our result, but we solely consider convex potentials and the fronts we find are supersonic, conservative, and monotone with constant asymptotic states, see Figure 2. For such potentials, the only previous result concerning fronts we are aware of is the bifurcation result by Iooss in [Ioo00] for supersonic fronts of small amplitude connecting constant states near a convex-concave turning point of  $\Phi'$ . A physical interpretation of these solutions is a deformation of the solid or crystal, though the fronts can travel in either direction for the same asymptotic states. Related 'pulsating' travelling waves have been studied in [IJ05]. Here the profile of the wave changes periodically while moving and the asymptotic states are wave trains. It was shown that in the truncated normal form on the centre manifold, pulsating front solutions bifurcate from convex-concave turning points of  $\Phi'$ .

The analytical investigations in this paper are motivated by the numerical simulations of atomistic Riemann problems which have recently been studied by the authors in [HR08]. We observed fronts in numerical simulations of (1) even for initial data that are far from the data of a front, see Figure 2. Hence, fronts are dynamically stable and provide fundamental building blocks for atomistic Riemann solvers.

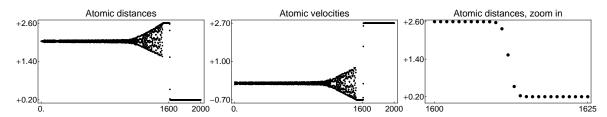


Figure 2: Fronts appear in the numerical simulations of FPU chains: snapshots of the atomic data with monotone front around particle  $\alpha = 1613$ .

The main result of this paper is the following.

**Theorem 1.1.** For all convex and smooth potentials  $\Phi$  the following assertions are satisfied:

- 1. Each front in the chain corresponds to a conservative shock in the p-system.
- 2. For each supersonic conservative shock in the p-system that satisfies a certain area condition there exists a corresponding monotone front in the chain.

Here 'correspond' means that shock and front have the same wave speed and asymptotic states.

The precise assertions of this theorem depend on the set of turning points of  $\Phi'$ :

- 1. If  $\Phi'$  has no turning points, then all shocks are non-conservative and fronts do not exist.
- 2. For strictly convex-concave  $\Phi'$  all conservative shocks are supersonic and satisfy the area condition. In this case Theorem 1.1 implies that *each* conservative shock can be realised by an atomistic front. In particular, this allows for arbitrary large jumps between the asymptotic states and extends the bifurcation result from [Ioo00].
- 3. For strictly concave-convex  $\Phi'$  all conservative shocks are subsonic and Theorem 1.1 does not imply an existence result for fronts.
- 4. If  $\Phi'$  has more than one turning point, then Theorem 1.1 provides the existence of fronts for a proper subset of all conservative shocks.

We emphasise that Theorem 1.1 does not imply the uniqueness of fronts with prescribed asymptotic states. Moreover, not every conservative shocks in the p-system corresponds to a front in the FPU chain. For functions  $\Phi'$  with one turning point the simulations in [HR08] rather suggest that only supersonic shocks allow for an atomistic realization as a (dynamically stable) front. This is supported by the bifurcation result in [Ioo00], which in fact disproves the existence of subsonic conservative shocks with small jump heights, and our results, which imply that subsonic shocks cannot minimize the action, compare the discussion at the end of §3.

We also mention the results about atomistic fronts by Aubry and Proville. In [AP07] they study FPU chains with concave  $\Phi'$  – so all shocks in the p-system are non-conservative – and allow for atomistic fronts by adding some damping force that respects uniform motion. By numerical simulations they found oscillations in the tails of such fronts and observed that these oscillations persist when the damping tends to zero. We therefore expect that non-conservative shock data can be related to heteroclinic connections of wave trains.

The proof of the first part of Theorem 1.1 is fairly straightforward and contained in Lemma 2.1 below. Proving the second part, which is mainly contained in Theorem 3.14, requires a number of preparatory steps, and uses the convexity of  $\Phi$ , the supersonic front speed, and the area condition in various fundamental steps. To guide the reader we give an overview of the key ideas and steps for the proof.

- 1. We use the a priori knowledge of the front speed in order to reformulate the problem as a nonlinear fixed point equation for a suitably normalised profile.
- 2. We identify an action functional for the deviation from the discontinuous shock profile such that the fixed point equation is the corresponding Euler-Lagrange equation.
- 3. We use the invariance of the set of monotone profiles under the gradient flow of the Lagrangian to connect stationary points in this set with fronts.
- 4. We establish bounds for the action functional and use the direct approach to show that the Lagrangian attains its minimum in the set of monotone profiles.

This paper is organised as follows. In §2 we give a more formal background for fronts and shocks of the p-system, and §3 contains the proof of the existence result. In §4 we prove that these fronts decay exponentially to their asymptotic states; the proof also applies to supersonic solitons with monotone tails and extends the known results there. In addition, we discuss numerical computations based on the gradient flow, and hereby illustrate the role of area condition, supersonic front speed, and energy conservation.

### 2 Fronts, shocks and normalisation

For our purposes it is convenient to use the atomic distances  $r_{\alpha} = x_{\alpha+1} - x_{\alpha}$  and velocities  $v_{\alpha} = \dot{x}_{\alpha}$  as the basic variables, changing (1) to the system

$$\dot{r}_{\alpha} = v_{\alpha+1} - v_{\alpha}$$
,  $\dot{v}_{\alpha} = \Phi'(r_{\alpha}) - \Phi'(r_{\alpha-1})$ .

Travelling waves are exact solutions to the infinite chain (1) that depend on a single phase variable  $\varphi = \alpha - \sigma t$ , where the *speed*  $\sigma$  equals the phase velocity. In terms of atomic distances and velocities travelling waves can be written as

$$r_{\alpha}(t) = R(\varphi), \qquad v_{\alpha}(t) = V(\varphi),$$

where the profile functions R and V solve the advance-delay differential equations

$$\sigma \frac{\mathrm{d}}{\mathrm{d}\varphi} R(\varphi) + V(\varphi + 1) - V(\varphi) = 0, \qquad \sigma \frac{\mathrm{d}}{\mathrm{d}\varphi} V(\varphi) + \Phi'(R(\varphi)) - \Phi'(R(\varphi - 1)) = 0, \tag{2}$$

which imply the energy law

$$\sigma \frac{\mathrm{d}}{\mathrm{d}\varphi} \left( \frac{1}{2} V^2(\varphi) + \Phi(R(\varphi)) \right) + \Phi' \left( R(\varphi) \right) V(\varphi + 1) - \Phi' \left( R(\varphi - 1) \right) V(\varphi) = 0. \tag{3}$$

The travelling waves in our context are *fronts*, which connect two different constant asymptotic states for  $\varphi \to -\infty$  and  $\varphi \to \infty$ , i.e.,

$$R, V \in \mathsf{C}^1 \cap \mathsf{L}^\infty \quad \text{with} \quad R(\varphi) \xrightarrow{\varphi \to \pm \infty} r_{\pm} \quad \text{and} \quad V(\varphi) \xrightarrow{\varphi \to \pm \infty} v_{\pm},$$
 (4)

where  $L^p$  and  $C^k$  denote the usual function spaces on the real line. The other variants of travelling waves mentioned in the introduction are *wave trains*, with periodic R and V, and *solitons*, that are localised over a constant background state, i.e.,  $r_+ = r_-$  and  $v_+ = v_-$ .

In [Ioo00] it has been proven that fronts bifurcate from turning points  $r_*$  of  $\Phi'$  with  $\Phi^{(4)}(r_*) \neq 0$  if and only if  $\Phi^{(4)}(r_*) < 0$ . These fronts have strictly monotone profiles that converge exponentially to their asymptotic states. Our main existence result extends this in the sense that we prove existence of fronts for any left and right states that satisfy certain constraints and can have large amplitude.

As a first result we establish necessary conditions for the existence of fronts, which reflect that each front converges to a shock in a large-scale limit. These conditions turn out to be the jump conditions for an energy conserving shock of the p-system (see below), and show that the speed  $\sigma$  of a front is completely determined by its asymptotic states.

For any atomic observable  $\psi = \psi(r, v)$  we define the mean and the jump by

$$\langle \psi \rangle := \tfrac{1}{2} \big( \psi(r_+, \, v_+) + \psi(r_-, \, v_-) \big) \quad \text{and} \quad [\![\psi]\!] := \psi(r_+, \, v_+) - \psi(r_-, \, v_-),$$

respectively, where  $r_{\pm}$  and  $v_{\pm}$  denote the asymptotic values of a front, see (4).

**Lemma 2.1.** Suppose that R and V as in (4) solve the front equation (2). Then,

$$\sigma[\![r]\!] + [\![v]\!] = 0, \qquad \sigma[\![v]\!] + [\![\Phi'(r)]\!] = 0, \qquad \sigma[\![\frac{1}{2}v^2 + \Phi(r)]\!] + [\![\Phi'(r)v]\!] = 0. \tag{5}$$

*Proof.* Integrate  $(2)_1$  over a finite interval [-n, n] gives

$$\sigma(R(n) - R(-n)) = -\int_{-n+1}^{n+1} V(\varphi) d\varphi + \int_{-n}^{n} V(\varphi) d\varphi = \int_{-n}^{-n+1} V(\varphi) d\varphi - \int_{n}^{n+1} V(\varphi) d\varphi,$$

and the limit  $n \to \infty$  yields  $(5)_1$ . The jump conditions  $(5)_2$  and  $(5)_3$  follow similarly from  $(2)_2$  and (3).

We mention that the jump conditions (5) are also derived in [AP07] and that a similar method is used in [Ser07] to derive jump conditions from purely discrete front equations.

#### 2.1 The p-system and conservative shocks

The p-system can be formally derived from the FPU chain as a continuum limit in the *hyperbolic scaling* of the *microscopic* coordinates t and  $\alpha$ . This scaling bridges to the *macroscopic* time  $\overline{t} = \varepsilon t$  and particle index  $\overline{\alpha} = \varepsilon \alpha$ , where  $0 < \varepsilon \ll 1$  is the scaling parameter. It is natural to scale the atomic positions in the same way, i.e.  $\overline{x} = \varepsilon x$ , which leaves atomic distances and velocities scale invariant.

Substituting an ansatz of macroscopic fields  $r(\overline{t}, \overline{\alpha})$  and  $v(\overline{t}, \overline{\alpha})$  such that  $r_{\alpha}(t) = r(\varepsilon t, \varepsilon \alpha)$ ,  $v_{\alpha}(t) = v(\varepsilon t, \varepsilon \alpha)$  into (1) and taking the limit  $\varepsilon \to 0$  yields the macroscopic conservation laws for mass and momentum

$$\partial_{\overline{t}}r - \partial_{\overline{\alpha}}v = 0, \qquad \partial_{\overline{t}}v - \partial_{\overline{\alpha}}\Phi'(r) = 0,$$
 (6)

which is the aforementioned p-system. It is well known that the p-system is hyperbolic if and only if  $\Phi$  is convex, and that for smooth solutions the energy is conserved via

$$\partial_{\overline{t}} \left( \frac{1}{2} v^2 + \Phi(r) \right) - \partial_{\overline{\alpha}} \left( v \Phi'(r) \right) = 0.$$

Next we summarise some facts about shocks in the p-system. For more details we refer to standard textbooks [Smo94, Daf00, LeF02], and to [HR08] for conservative shocks.

A shock connecting a left state  $u_- = (r_-, v_-)$  to a right state  $u_+ = (r_+, v_+)$  propagates with a constant shock speed  $\sigma$  so that  $u_-$  and  $u_+$  satisfy the Rankine-Hugeniot jump conditions for mass and momentum  $(5)_1$  and  $(5)_2$ . Corresponding to the two characteristic velocities of (6) one distinguishes between 1-shocks with  $\sigma < 0$  and 2-shocks with  $\sigma > 0$ .

An important observation is that for either convex or concave flux  $\Phi'$  the jump conditions  $(5)_1$  and  $(5)_2$  imply that the jump condition for the energy  $(5)_3$  must be violated, that means

$$\sigma[\![\frac{1}{2}v^2 + \Phi(r)]\!] + [\![v\,\Phi'(r)]\!] \neq 0. \tag{7}$$

For non-convex or non-concave  $\Phi'$ , however, it is possible to find *conservative shocks* that satisfy all three jump conditions from (5), see Theorem 5.1 in [HR08]. Eliminating  $\llbracket v \rrbracket$  and  $\sigma$  in (5) shows that each conservative shock satisfies

$$\mathcal{J}(r_{-}, r_{+}) := \|\Phi(r)\| - \|r\| \langle \Phi'(r) \rangle = 0. \tag{8}$$

Conversely, for each solution to (8) there exist, up to Galilean transformations, exactly two corresponding conservative shocks which differ only in  $\operatorname{sgn}[v] = -\operatorname{sgn} \sigma$  and propagate in opposite directions. The geometric interpretation of (8) is that the signed area between the graphs of  $\Phi'$  and the secant line through  $\Phi'(r_-)$  and  $\Phi'(r_+)$  is zero over  $[r_-, r_+]$ , compare Figure 4 below.

For the harmonic potential  $\Phi(r) = \frac{c}{2}r^2$  the p-system is linearly degenerate, hence all shocks are conservative. In the nonlinear case, however, the solution set to (8) is either empty or the union of curves in the  $(r_-, r_+)$ -plane, see Figure 3 for an example. In particular, precisely from turning points of  $\Phi'$  there bifurcate curves of conservative shocks, see [HR08].

Shocks come in different types determined by the relation of the shock speed  $\sigma$  and the sound speeds  $\lambda(r) := \pm \sqrt{\Phi''(r)}$  evaluated in  $r_-$  and  $r_+$ , where the signs of both the sound speed and the shock speed are taken negative (positive) when considering 1-shocks (2-shocks). More precisely, a shock connecting  $u_-$  to  $u_+$  with speed  $\sigma$  is called

- 1. compressive, or Lax shock, if  $\lambda(r_{-}) > \sigma > \lambda(r_{+})$ ,
- 2. rarefaction shock, if  $\lambda(r_{-}) < \sigma < \lambda(r_{+})$ ,
- 3. supersonic, or fast undercompressive, if  $|\sigma| > |\lambda(r_{-})|$  and  $|\sigma| > |\lambda(r_{+})|$ ,
- 4. subsonic, or slow undercompressive, if  $|\sigma| < |\lambda(r_-)|$  and  $|\sigma| < |\lambda(r_+)|$ ,
- 5. sonic, if  $|\sigma| = |\lambda(r_-)|$  or  $|\sigma| = |\lambda(r_+)|$ .

For all sufficiently small jump heights  $|r_+ - r_-| + |v_+ - v_-|$  one can show that compressive and rarefaction shocks have negative and positive, respectively, energy production in (7). Consequently, all conservative shocks with small jump height are either sonic or undercompressive. The conservative shocks bifurcating from turning points  $r_*$  of  $\Phi'$  are supersonic if  $\Phi^{(4)}(r_*) < 0$  and subsonic if  $\Phi^{(4)}(r_*) > 0$ , see [HR08].

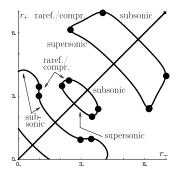


Figure 3: Conservative shocks for the potential  $\Phi(r+1) = r + \frac{1}{2}r^2 + \frac{1}{20}r^3 - \frac{1}{4}\cos(2r) + \frac{1}{10}\sin(3r)$ : solid lines form the solution set to  $\mathcal{J}(r_-, r_+) = 0$ , i.e., the distance data for conservative shocks; bullets lie at local extrema of the curves in the coordinate directions, and are the points where the shock type changes.

#### 2.2 Normalisation and reformulation

Next we show that, after a suitable renormalisation, the front equations for R and V are equivalent to a nonlinear fixed point equation for a normalised profile W with asymptotic states  $\pm 1$ . To this end we introduce the averaging operator

$$(\mathcal{A}U)(\varphi) := \int_{\varphi - \frac{1}{2}}^{\varphi + \frac{1}{2}} U(\tilde{\varphi}) \, \mathrm{d}\tilde{\varphi},$$

which satisfies

$$\frac{\mathrm{d}}{\mathrm{d}\varphi}(\mathcal{A}U) = \nabla U := U\left(\cdot + \frac{1}{2}\right) - U\left(\cdot - \frac{1}{2}\right), \qquad \lim_{\varphi \to \pm \infty} (\mathcal{A}U)(\varphi) = \lim_{\varphi \to \pm \infty} U(\varphi). \tag{9}$$

For given asymptotic front states  $(r_{\pm}, v_{\pm})$  we further introduce a normalised potential  $\widehat{\Phi}$  by

$$\widehat{\Phi}(w) = \frac{4}{[\![\Phi'(r)]\!][\![r]\!]} \Phi\left(\langle r \rangle + \frac{1}{2} [\![r]\!] w\right) - \frac{2\langle \Phi'(r) \rangle}{[\![\Phi'(r)]\!]} w,$$

which is convex on [-1, 1] and strictly convex if  $\Phi$  is. Moreover, the jump conditions from (5) imply  $\Phi'(\pm 1) = \pm 1$  and  $\widehat{\Phi}(1) = \widehat{\Phi}(-1)$ , and the shock corresponding to  $(r_{\pm}, v_{\pm})$  is supersonic if and only if  $\widehat{\Phi}''(1) < 1$  and  $\widehat{\Phi}''(-1) < 1$ .

**Lemma 2.2.** For fixed asymptotic states  $(r_{\pm}, v_{\pm})$  there is a one-to-one correspondence between front solutions to (2) and solutions W to

$$W = \mathcal{A}\widehat{\Phi}'(\mathcal{A}W),\tag{10}$$

with  $W(\varphi) \xrightarrow{\varphi \to \pm \infty} \pm 1$ .

*Proof.* Suppose that R and V solve (2). Then there exists a normalised profile W such that

$$V = \langle v \rangle + \frac{1}{2} \llbracket v \rrbracket W. \tag{11}$$

By (9) the first equation from (2) is equivalent to

$$-\sigma \widehat{R} = AV + c = \langle v \rangle + \frac{1}{2} [v] AW + c$$

with  $\widehat{R}(\varphi) = R(\varphi - \frac{1}{2})$  and an integration constant c. Passing to  $\varphi \to -\infty$  and  $\varphi \to \infty$  we find

$$-\sigma [\![ r]\!] = [\![ v]\!], \quad c = -\sigma \langle r \rangle - \langle v \rangle,$$

and this gives

$$\widehat{R} = \langle r \rangle + \frac{1}{2} \llbracket r \rrbracket \mathcal{A} W. \tag{12}$$

The second equation from (2) transforms into

$$-\sigma V = \mathcal{A}\Phi'(\widehat{R}) + d,\tag{13}$$

and inspecting the asymptotic values we find

$$-\sigma[\![v]\!] = [\![\Phi'(r)]\!], \quad d = -\sigma\langle v\rangle - \langle \Phi'(r)\rangle. \tag{14}$$

Inserting (11) and (12) into (13) gives

$$W = -\frac{2}{\sigma \|v\|} \mathcal{A} \Big( \Phi' \Big( \langle r \rangle + \frac{1}{2} \|r\| \mathcal{A} W \Big) - \langle \Phi'(r) \rangle \Big),$$

which is (10) due to (14). Finally, it is easy to see that each solution to (10) determines a front via (11) and (12).  $\Box$ 

The equivalence between the lattice equation (2) for travelling waves and the nonlinear eigenvalue problem  $\sigma^2 W = \mathcal{A}\widehat{\Phi}'(\mathcal{A}W)$  is well established for wave trains and solitons, compare for instance [FW94, FV99], but in the case of fronts we have not seen this formulation before. An important difference is that for fronts the speed  $\sigma$  is completely determined by the asymptotic states and can hence be removed from the problem.

We conclude with some remarks concerning the regularity of fronts. Suppose that  $W \in L^{\infty}$  solves (10). Using (9), compare also Lemma 3.3 below, and the smoothness of  $\Phi$  we find

$$\frac{\mathrm{d}^2}{\mathrm{d}\omega^2}W = \nabla \left[\widehat{\Phi}''(\mathcal{A}W)\nabla W\right],\tag{15}$$

and hence  $W \in W^{2,\infty} \subset C$ . Moreover, we infer that  $W \in C^2$  and, differentiating (15) further, that W is as smooth as  $\Phi$ . Finally, exploiting (11) and (12) we arrive at the following result and refer to §4.1 for further qualitative properties of fronts.

**Remark 2.3.** Each solution  $W \in L^{\infty}$  to (10) is contained in  $C^2$  and provides a smooth solution to (2) with at least  $R, V \in C^2 \cap L^{\infty}$ .

### 3 Proof of the existence result

In order to prove the existence of monotone solutions W to the fixed point problem (10) we consider only normalised potentials  $\Phi = \widehat{\Phi}$  and rely on the following standing assumption. This involves the function

$$g_{\Phi}(w) := \int_{-\infty}^{w} v - \Phi'(v) \, dv = \Phi(-1) - \Phi(w) + \frac{1}{2}w^2 - \frac{1}{2}, \tag{16}$$

which measures the signed area between the identity and the graph of  $\Phi'$ , see Figure 4.

**Assumption 3.1.** The potential  $\Phi$  satisfies

- (R) regularity:  $\Phi$  is twice continuously differentiable on [-1, 1],
- (N) normalisation:  $\Phi'(-1) = -1$  and  $\Phi'(1) = 1$ ,
- (C) convexity:  $\Phi''$  is nonnegative on [-1, 1],

- (E) conservation of energy:  $\Phi(-1) = \Phi(1)$ ,
- (S) supersonic front speed:  $\Phi''(-1) < 1$  and  $\Phi''(1) < 1$ .
- (A) positive signed area:  $g_{\Phi}(w) > 0$  for all  $w \in (-1, 1)$ .

We mention that (N) and (R) are made for convenience, (E) is necessary according to Lemma 2.1, and (C) is needed for the monotonicity of fronts. The status of (S) and (A) is more delicate: If  $\Phi'$  has only one turning point, then (S) coincides with the bifurcation condition in [Ioo00] and implies (A), see Remark 3.2 below. If  $\Phi'$  has more than one turning point, then (A) is independent of (S). In any case both (S) and (A) are closely related to the existence of action-minimising fronts as discussed in more detail at the end of §3 and illustrated in §4.2.

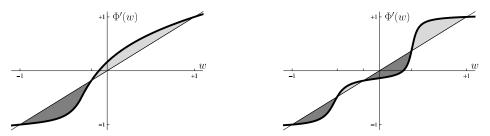


Figure 4: Two examples for force functions  $\Phi'$  that satisfy Assumption 3.1; the first one is prototypical for the supersonic fronts with small amplitudes that bifurcate from convex-concave turning points. Condition (A) precisely means that for each -1 < w < 1 the signed area between the identity and the graph of  $\Phi'$  is positive in the stripe [-1, w]; the signed area vanishes in the stripe [-1, 1] if and only if the corresponding p-system shock conserves the energy via (E).

Recall that turning points of  $\Phi'$  are exactly those points in which  $\Phi''$  changes its monotonicity. More precisely, convex-concave (concave-convex) turning points correspond to local maximisers (minimiser) of  $\Phi''$ . We now summarize the main observations concerning the turning points of  $\Phi'$ .

**Remark 3.2.** Suppose that (N), (R), and (S) are satisfied. Then  $\Phi'$  has at least one convex-concave turning point in (-1, 1). Moreover, if  $\Phi'$  has no further turning point in (-1, 1) then (E) implies (A).

Proof. Suppose for contradiction that  $\max \Phi''|_{[-1,1]} \le 1$ . Then, for all  $w \in [-1,1]$  we find  $g''_{\Phi}(w) = 1 - \Phi''(w) \ge 0$  and hence  $0 = g'_{\Phi}(-1) \le g_{\Phi}'(w) \le g_{\Phi}'(+1) = 0$ . This implies  $g'_{\Phi}(w) = 0$  for all  $w \in [-1,1]$ , and hence a contradiction to (S). Therefore,  $\Phi''$  possesses a local maximiser  $w \in (-1,1)$ , which is a convex-concave turning point of  $\Phi'$ .

Towards (A) suppose additionally (E) and that  $\Phi'$  is convex-concave in [-1, 1]. Then,  $g_{\Phi}(1) = g_{\Phi}(-1) = 0$ , and the monotonicity properties of  $\Phi''$  imply that there exist  $-1 \le w_1 \le w_2 \le 1$  such that  $\Phi''(w) \le 1$  and  $\Phi''(w) \ge 1$  for all  $w \in I_1 = [-1, w_1] \cup [w_2, 1]$  and  $w \in I_2 = [w_1, w_2]$ , respectively. In particular,  $g_{\Phi}$  is convex in  $I_1$  but concave in  $I_2$ , and combining this with  $0 = g_{\Phi}(\pm 1) = g'_{\Phi}(\pm 1)$  and  $g''_{\Phi}(\pm 1) > 0$ , we readily find  $g_{\Phi}(w) > 0$  for all  $w \in (-1, +1)$ .

#### 3.1 The action functional

In this section we cast the problem in a variational framework and show that

$$W = \mathcal{T}[W], \qquad \mathcal{T}[W] := \mathcal{A}\Phi'(\mathcal{A}W),$$

is the Euler-Lagrange equation for an action integral. To this end we introduce the affine Banach space

$$\mathcal{H}:=\Big\{\text{functions }W:\mathbb{R}\to\mathbb{R}\text{ such that }\widetilde{W}=W_{\text{sh}}-W\in\mathsf{L}^2\Big\},$$

where the reference profile  $W_{\rm sh}(\varphi) = {\rm sgn}(\varphi)$  is the shock profile that connects -1 to 1. We also define the Lagrangian on  $\mathcal{H}$  by

$$\mathcal{L}(W) = \int_{\mathbb{R}} L(W, \mathcal{A}W) - L(W_{\rm sh}, \mathcal{A}W_{\rm sh}) \,\mathrm{d}\varphi, \quad L(v, r) = \frac{1}{2}v^2 - \Phi(r), \tag{17}$$

and a formal calculation shows  $\partial \mathcal{L}[W] = W - \mathcal{T}[W]$ . Notice that the ansatz  $\widetilde{W} \in \mathsf{L}^2$  arises naturally when computing the asymptotic behaviour for  $\varphi \to \pm \infty$ . In fact, since  $\widetilde{AW}$  decays like  $\widetilde{W}$  and due to  $\Phi'(\pm 1) = -1$  the integrand in (17) behaves like  $\frac{1}{2}(1 - \Phi''(\pm 1))\widetilde{W}(\varphi)^2$ .

In the remainder of this section we show that both  $\mathcal{L}$  and  $\mathcal{T}$  are well-defined on  $\mathcal{H}$ . We start with some properties of the averaging operator  $\mathcal{A}$  that are proven in [Her09].

**Lemma 3.3.** The linear operator A is well-defined on  $L^p$ ,  $1 \le p \le \infty$ , and has the following properties:

- 1. A maps into  $W^{1,p}$  with  $(AW)'(\varphi) = W(\varphi + 1/2) W(\varphi 1/2)$ ,
- 2.  $\mathcal{A}$  maps  $\mathsf{L}^2$  into  $\mathsf{L}^2 \cap \mathsf{L}^{\infty}$  with  $\|\mathcal{A}\widetilde{W}\|_{\infty} \leq \|\widetilde{W}\|_2$  and  $\|\mathcal{A}\widetilde{W}\|_2 \leq \|\widetilde{W}\|_2$ ,
- 3. A is self-adjoint on  $L^2$ ,
- 4. If a sequence  $(\widetilde{W}_n)_n$  converges weakly in  $L^2$  to some limit  $\widetilde{W}_{\infty}$ , then  $(\widetilde{AW}_n)_n$  converges strongly and pointwise to  $\widetilde{AW}_{\infty}$  in  $L^2([-M, M])$  for each  $M < \infty$ .

Our next result shows  $\mathcal{T}[W] - W \in L^2$  for all  $W \in \mathcal{H}$  and implies that  $\mathcal{T} : \mathcal{H} \to \mathcal{H}$  is well-defined.

**Lemma 3.4.** For any  $W \in \mathcal{H}$  we have

$$W - \Phi'(\mathcal{A}W) \in L^2, \qquad W - \mathcal{A}\Phi'(\mathcal{A}W) \in L^2,$$
 (18)

as well as

$$\int_{\mathbb{R}} W\mu - \Phi'(\mathcal{A}W)\mathcal{A}\mu \,d\varphi = \int_{\mathbb{R}} W\mu - \mathcal{A}\Phi'(\mathcal{A}W)\mu \,d\varphi \tag{19}$$

for all test functions  $\mu \in L^2$ .

Proof. With

$$\left|\Phi'\left((\mathcal{A}W)(\varphi)\right) - \Phi'\left((\mathcal{A}W_{\mathrm{sh}})(\varphi)\right)\right| \le C\left|\widetilde{\mathcal{A}W}(\varphi)\right|, \quad C = \sup\left\{\left|\Phi''(w)\right| : \left|w\right| \le \max\{1, \|\mathcal{A}W\|_{\infty}\}\right\}$$

for all  $\varphi$ , and  $\Phi'(\mathcal{A}W_{\rm sh}(\varphi)) = W_{\rm sh}(\varphi)$  for  $|\varphi| \geq \frac{1}{2}$ , we find (with the usual cut-off function  $\chi$ )

$$\left| W - \Phi'(\mathcal{A}W) \right| \le \widetilde{W} + \chi_{\left[-\frac{1}{2}, \frac{1}{2}\right]} \left| W_{\rm sh} - \Phi'(\mathcal{A}W_{\rm sh}) \right| + C \left| \mathcal{A}\widetilde{W} \right|.$$

This gives  $(18)_1$  since  $\widetilde{W}$ ,  $\widetilde{AW} \in L^2$ , and the proof of  $(18)_2$  is similar. Now let M > 0 be arbitrary. Since  $\mathcal{A}$  is symmetric, see Lemma 3.3, we write

$$\int_{-M}^{M} \Phi'(\mathcal{A}W) \mathcal{A}\mu \, d\varphi = \int_{\mathbb{R}} \mu \mathcal{A}(\chi_{[-M,M]} \Phi'(\mathcal{A}W)) \, d\varphi = \int_{-M}^{M} \mu \mathcal{A}\Phi'(\mathcal{A}W) \, d\varphi + E_M, \tag{20}$$

where the error term satisfies

$$|E_M| \le C \begin{pmatrix} M + \frac{1}{2} & -M + \frac{1}{2} \\ \int_{M - \frac{1}{2}} |\mu| \, d\varphi + \int_{-M - \frac{1}{2}} |\mu| \, d\varphi \end{pmatrix}, \qquad C = \sup \{ |\Phi'(w)| : |w| \le ||AW||_{\infty} \}.$$

Finally, we add  $\int_M^M W \mu \, d\varphi$  on both sides of (20), and taking the limit  $M \to \infty$  yields (19).

We now prove that  $\mathcal{L}$  is well-defined and Gâteaux-differentiable on  $\mathcal{H}$ .

**Remark 3.5.** For each  $w_0$  the pointwise normalised potential

$$\Phi_{w_0}(w) := \Phi(w_0 + w) - \Phi'(w_0)w - \Phi(w_0)$$

satisfies  $0 \le \Phi_{w_0}(w) \le \frac{c}{2} w^2$  with  $c = \sup \Phi''|_{[w_0, w]}$ .

**Lemma 3.6.** The functional  $\mathcal{L}$  is well-defined on  $\mathcal{H}$ . Moreover, it is Gâteaux differentiable with locally Lipschitz continuous derivative  $\partial \mathcal{L}[W] = W - \mathcal{T}[W]$ .

*Proof.* By construction, we have

$$L(W, \mathcal{A}W) - L(W_{\rm sh}, \mathcal{A}W_{\rm sh}) = \frac{1}{2}\widetilde{W}^2 - W_{\rm sh}\widetilde{W} + \Phi'(\mathcal{A}W_{\rm sh})\mathcal{A}\widetilde{W} - \Phi_{\mathcal{A}W_{\rm sh}}(\mathcal{A}\widetilde{W})$$

with pointwise normalised potentials  $\Phi_{AW_{sh}}$  as in Remark 3.5. Using (19) with  $W = W_{sh}$  and  $\mu = \widetilde{W}$  we find

$$\int_{\mathbb{R}} W_{\rm sh} \widetilde{W} - \Phi'(\mathcal{A}W_{\rm sh}) \mathcal{A}\widetilde{W} \, d\varphi = \int_{\mathbb{R}} \left( W_{\rm sh} - \mathcal{A}\Phi'(\mathcal{A}W_{\rm sh}) \right) \widetilde{W} \, d\varphi,$$

with well-defined integrals on both sides. Using  $C := \sup \Phi''|_{[-1,1]} < \infty$  we estimate

$$\int_{\mathbb{R}} \frac{1}{2} \widetilde{W}^2 \, d\varphi < \infty, \quad \int_{\mathbb{R}} \Phi_{\mathcal{A}W_{sh}}(\mathcal{A}\widetilde{W}) \, d\varphi \leq C \, \|\mathcal{A}\widetilde{W}\|_2^2 \leq C \, \|\widetilde{W}\|_2^2,$$

and conclude that  $\mathcal{L}(W)$  is well-defined for all  $W \in \mathcal{H}$ . Moreover, (18) implies  $W - \mathcal{T}[W] \in \mathsf{L}^2$ , and in view of (19) we readily verify the formula for  $\partial \mathcal{L}$  as well as the claimed Lipschitz property.

#### 3.2 Monotone and heteroclinic functions

In order to introduce a refined ansatz space for the front profile W we start with some preliminary remarks concerning the weak formulation of monotonicity, asymptotic values, and  $\mathsf{L}^\infty$  bounds.

Let  $[\varphi_0, \infty)$  be some interval,  $U \in \mathsf{L}^\infty([\varphi_0, \infty))$  be fixed, and let  $\mu \geq 0$  denote an arbitrary smooth test function with compact support in  $(\varphi_0, \infty)$ . Then, the function U is said to

- 1. be increasing, if  $\int_{\mathbb{R}} (U(\varphi + \bar{\varphi}) U(\varphi))\mu(\varphi) d\varphi \geq 0$  for all shifts  $\bar{\varphi} \geq 0$  and all  $\mu$ ,
- 2. be nonnegative, if  $\int_{\mathbb{R}} U(\varphi)\mu(\varphi) d\varphi \geq 0$  for all  $\mu$ ,
- 3. take values in  $[u_1, u_2]$ , if  $u_2 \ge \int_{\mathbb{R}} U(\varphi)\mu(\varphi) d\varphi \ge u_1$  for all  $\mu \ge 0$  with  $\int_{\mathbb{R}} \mu(\varphi) d\varphi = 1$ ,
- 4. have the asymptotic value  $u_+$  for  $\varphi \to \infty$ , if  $\int_{\mathbb{R}} U(\varphi + \bar{\varphi})\mu(\varphi) d\varphi \to u_+ \int_{\mathbb{R}} \mu(\varphi) d\varphi$  as  $\bar{\varphi} \to \infty$  for all  $\mu$ .

Note that all these properties are preserved under weak convergence, and that similar statements hold on  $(\infty, \varphi_0]$ .

We aim at establishing the existence of fronts in the convex set

$$\mathcal{C} := \left\{ W \in \mathcal{H} \text{ is increasing with } W(\varphi) \to \pm 1 \text{ as } \varphi \to \pm \infty, \right\}$$

where the convergence conditions mean that W has asymptotic values -1 and +1 in the above sense.

A particular problem in our subsequent analysis is to control the relative shift between a profile function W and the reference profile  $W_{\rm sh}$ . For this reason we introduce the set of all pinned profile functions by

$$\mathcal{C}_0 := \left\{ W \in \mathcal{C} \text{ with } \begin{array}{l} W|_{[0,+\infty)} \text{ takes values in } [0,+1] \\ W|_{(-\infty,0]} \text{ takes values in } [-1,0] \end{array} \right\}$$

Obviously, for each  $W \in \mathcal{C}$  there exists a phase shift  $\varphi_0$  such that  $W(\cdot - \varphi_0) \in \mathcal{C}_0$ , and this phase shift is unique if W is strictly increasing. Moreover, we have  $W \in \mathcal{C}_0$  if and only if  $\widetilde{W} \in \widetilde{\mathcal{C}}_0$  with

$$\widetilde{\mathcal{C}}_0 := \left\{ \widetilde{W} \in \mathsf{L}^2 \text{ such that } \begin{array}{l} \widetilde{W}|_{[0,+\infty)} \text{ is decreasing with values in } [0,+1] \\ \widetilde{W}|_{(-\infty,\,0]} \text{ is decreasing with values in } [-1,\,0] \end{array} \right\}.$$

Notice that the set  $\widetilde{\mathcal{C}}_0$  is convex and closed under weak convergence in  $\mathsf{L}^2$ .

### 3.3 Variational approach

The starting point for our variational existence result is the invariance of  $\mathcal{C}$  under the action of  $\mathcal{T}$ . In fact, it is straightforward that the averaging operator  $\mathcal{A}$  respects both the monotonicity and asymptotic values of W. In addition, since  $\Phi'$  is a monotone map on [-1, 1] with  $\Phi'(\pm 1) = \pm 1$  the set  $\mathcal{C}$  is also invariant under the pointwise application of  $\Phi'$ . Notice, however, that  $\mathcal{C}_0$  is *not* invariant under the action of  $\mathcal{T}$  since for (continuous) W with W(0) = 0 in general we have  $\mathcal{T}[W](0) \neq 0$ .

Next we consider the gradient flow of  $\mathcal{L}$  in  $\mathcal{H}$ , that is

$$\frac{\mathrm{d}}{\mathrm{d}s}W = -\partial \mathcal{L}[W] = -W + \mathcal{T}[W] \tag{21}$$

with flow time s. According to Lemma 3.6, the initial value problem for this  $\mathcal{H}$ -valued ODE is well-defined, and we readily verify that

$$\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{L}(W) = \left\langle \partial \mathcal{L}(W), \frac{\mathrm{d}}{\mathrm{d}s}W \right\rangle = -\|W - \mathcal{T}[W]\|_2^2. \tag{22}$$

In particular, each stationary point of (21) is a fixed point of  $\mathcal{T}$ .

The key observation is that C is an invariant set for (21). To see this we introduce the corresponding Euler scheme with step size  $0 < \lambda < 1$ , that is

$$W \mapsto W - \lambda \partial \mathcal{L}[W] = (1 - \lambda)W + \lambda \mathcal{T}[W]. \tag{23}$$

This scheme leaves  $\mathcal{C}$  invariant because  $W \in \mathcal{C}$  implies  $\mathcal{T}[W] \in \mathcal{C}$ , and since  $\mathcal{C}$  is convex and closed in  $\mathcal{H}$  the claim follows with  $\lambda \to 0$ . As a consequence we obtain the following result.

**Lemma 3.7.** Each local minimiser of  $\mathcal{L}$  in  $\mathcal{C}$  is a solution to the front equation  $W = \mathcal{T}[W]$ .

We proceed with two remarks: (i) The front equation can be considered as the Euler-Lagrange equation for  $\mathcal{L}$  corresponding to variations  $W \rightsquigarrow W + \delta \widetilde{W}$  with arbitrary  $\widetilde{W} \in \mathsf{L}^2$ . Therefore, the fact that minimisers of  $\mathcal{L}$  in  $\mathcal{C}$  solve the front equation is not clear a priori but follows from of the invariance properties of  $\mathcal{C}$  and the dissipation inequality (22). (ii) There is no analogue to Lemma 3.7 for local maximisers. This follows from the next Remark and reflects that  $\mathcal{C}$  is not invariant under the negative gradient flow of  $\mathcal{L}$ .

**Remark 3.8.** The shock profile  $W_{\rm sh}$  is a local maximiser for  $\mathcal L$  in  $\mathcal C$  but does not satisfy the front equation.

*Proof.* Let  $W \in \mathcal{C}$  be arbitrary with  $W \neq W_{\rm sh}$ . For  $0 \leq \varepsilon \leq 1$  we define  $W_{\varepsilon} = (1 - \varepsilon)W_{\rm sh} + \varepsilon W$  and note that  $W_{\varepsilon} \in \mathcal{C}$ . Lemma 3.6 yields

$$\lambda := \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \mathcal{L}(W_{\varepsilon})|_{\varepsilon=0} = \langle \partial \mathcal{L}[W_{\mathrm{sh}}], W - W_{\mathrm{sh}} \rangle = -\int_{\mathbb{T}} (W_{\mathrm{sh}} - \mathcal{T}[W_{\mathrm{sh}}]) (W_{\mathrm{sh}} - W) \, \mathrm{d}\varphi.$$

On the one hand, we have  $\mathcal{T}[W_{\rm sh}] \in \mathcal{C}$  with  $W_{\rm sh}(\varphi) < \mathcal{T}[W_{\rm sh}](\varphi)$  for  $-1 < \varphi < 0$ ,  $W_{\rm sh}(\varphi) > \mathcal{T}[W_{\rm sh}](\varphi)$  for  $0 < \varphi < 1$ , and  $W_{\rm sh}(\varphi) = \mathcal{T}[W_{\rm sh}](\varphi)$  for  $|\varphi| \ge 1$ . On the other hand,  $W \in \mathcal{C}$  implies  $W_{\rm sh}(\varphi) \le W(\varphi)$  and  $W_{\rm sh}(\varphi) \ge W(\varphi)$  for  $\varphi < 0$  and  $\varphi > 0$ , respectively. From this we conclude  $\lambda \le 0$  and  $W \ne W_{\rm sh}$  gives  $\lambda < 0$ . Finally,  $W_{\rm sh}$  does not equal  $\mathcal{T}[W_{\rm sh}]$  as the latter is continuous.

Our strategy for proving the existence of fronts is to show that  $\mathcal{L}$  attains its minimum in  $\mathcal{C}$ . To this end we follow the direct approach, and prove that minimising sequences are precompact.

#### 3.4 Bounds for $\mathcal{L}$

Towards compactness results for minimising sequences for  $\mathcal{L}$  in  $\mathcal{C}$ , we first prove that corresponding sequences in  $\mathcal{C}_0$  also minimise  $\mathcal{L}$ . To this end we start with a technical result.

**Lemma 3.9.** Let  $U \in L^{\infty}$  be monotone with asymptotic values  $u_{-}$  and  $u_{+}$  for  $\varphi \to -\infty$  and  $\varphi \to \infty$ , respectively. Then we have

$$\int_{\mathbb{D}} U(\varphi + \bar{\varphi}) - U(\varphi) \, d\varphi = (u_{+} - u_{-})\bar{\varphi}.$$
(24)

for any phase shift  $\bar{\varphi}$ .

*Proof.* For M > 0 we compute

$$\int_{\mathbb{R}} \chi_{[-M,M]}(\varphi) \Big( U(\varphi + \bar{\varphi}) - U(\varphi) \Big) \, d\varphi = \int_{-M+\bar{\varphi}}^{M+\bar{\varphi}} U(\varphi) \, d\varphi - \int_{-M}^{M} U(\varphi) \, d\varphi = \int_{M}^{M+\bar{\varphi}} U(\varphi) \, d\varphi - \int_{-M}^{M+\bar{\varphi}} U(\varphi) \, d\varphi = \int_{M}^{M+\bar{\varphi}} U(\varphi) \, d\varphi = \int_{M}^{M+\bar{\varphi}}$$

Since the integrand on the left hand side has a sign and converges pointwise, we can pass to the limit  $M \to \infty$  by means of the Monotone Convergence Theorem, and this gives the desired result.

Notice that the proof of Lemma 3.9 is very close to that of Lemma 2.1, and that the assumptions on U can easily be weakened. For instance, (24) holds also for all functions  $U \in \mathsf{BV}$  as these can be written as the difference of two monotone functions with well defined asymptotic values.

Lemma 3.9 implies that  $\mathcal{L}$  is invariant under phase shifts, and hence  $\inf \mathcal{L}|_{\mathcal{C}} = \inf \mathcal{L}|_{\mathcal{C}_0}$ .

Corollary 3.10. For all  $W \in \mathcal{C}$  and all phase shifts  $\bar{\varphi}$  we have  $\mathcal{L}(W(\cdot + \bar{\varphi})) = \mathcal{L}(W)$ .

*Proof.* We define the monotone functions

$$U_1(\varphi) := \inf_{\tilde{\varphi} \geq \varphi} \frac{1}{2} W^2(\tilde{\varphi}), \quad U_2(\varphi) := -\inf_{\tilde{\varphi} \geq \varphi} \Phi((\mathcal{A}W)(\tilde{\varphi})), \quad U_3 := \frac{1}{2} W^2 - U_1, \quad U_4 := -\Phi(\mathcal{A}W) - U_2,$$

and find

$$\mathcal{L}(W(\cdot + \bar{\varphi})) - \mathcal{L}(W) = \sum_{i=1}^{4} \int_{\mathbb{R}} U_i(\varphi + \bar{\varphi}) - U_i(\varphi) \, d\varphi = \bar{\varphi}(\Phi(-1) - \Phi(1)) = 0$$
 (25)

thanks to Lemma 3.9.

Note that the energy condition (E) is essential for Corollary 3.10. In fact, if it is violated, then (25) implies that  $\mathcal{L}$  is unbounded from below and above.

Next we derive explicit bounds for  $\mathcal{L}(W)$  in terms of  $\|\widetilde{W}\|_2$  by comparing with the functional

$$\mathcal{L}_{\#}(W) := \int_{\mathbb{R}} L(W, W) - L(W_{\rm sh}, W_{\rm sh}) \, \mathrm{d}\varphi = \int_{\mathbb{R}} g_{\Phi}(W(\varphi)) \, \mathrm{d}\varphi, \tag{26}$$

where the last identity holds by definition of  $g_{\Phi}$ , see (16), and (E). In particular, (A) implies  $\mathcal{L}_{\#}(W) \geq 0$ .

**Lemma 3.11.** There exists a constant  $c \leq 4$  such that

$$|\mathcal{L}_{\#}(W) - \mathcal{L}(W)| \le c \tag{27}$$

for all  $W \in \mathcal{C}$ .

*Proof.* The monotonicity of  $W \in \mathcal{C}$  implies

$$W\left(\varphi - \frac{1}{2}\right) \le W(\varphi) \le W\left(\varphi + \frac{1}{2}\right), \quad W\left(\varphi - \frac{1}{2}\right) \le (\mathcal{A}W)(\varphi) \le W\left(\varphi + \frac{1}{2}\right)$$

for all  $\varphi \in \mathbb{R}$ , and due to  $|\Phi'(w)| \leq 1$  for all  $w \in [-1, 1]$  we also have

$$\left|\Phi((\mathcal{A}W)(\varphi)) - \Phi(W(\varphi))\right| \le \left|(\mathcal{A}W)(\varphi) - W(\varphi)\right|.$$

In combination we obtain

$$\left|\Phi\left((\mathcal{A}W)(\varphi)\right) - \Phi\left(W(\varphi)\right)\right| \le W\left(\varphi + \frac{1}{2}\right) - W\left(\varphi - \frac{1}{2}\right)$$

and Lemma 3.9 yields

$$\int_{\mathbb{R}} \left| \Phi \left( (\mathcal{A}W)(\varphi) \right) - \Phi \left( W(\varphi) \right) \right| \, \mathrm{d}\varphi \le 2. \tag{28}$$

Therefore,

$$|\mathcal{L}(W) - \mathcal{L}_{\#}(W)| \leq \int_{\mathbb{R}} \left| \Phi \left( (\mathcal{A}W)(\varphi) \right) - \Phi \left( W(\varphi) \right) \right| \, \mathrm{d}\varphi + \int_{\mathbb{R}} \left| \Phi \left( (\mathcal{A}W_{\mathrm{sh}})(\varphi) \right) - \Phi \left( W_{\mathrm{sh}}(\varphi) \right) \right| \, \mathrm{d}\varphi \leq 4,$$

where we used (28) both for W and  $W_{\rm sh}$ .

The following lemma is key to our approach and strongly relies on the signed are condition (A) and the monotonicity of all profiles  $W \in \mathcal{C}$ .

**Lemma 3.12.** There exist two constants  $\underline{c} > 0$  and  $\overline{c} > 0$  such that

$$\underline{c} \| \widetilde{W} \|_{2}^{2} \leq \mathcal{L}_{\#}(W) \leq \overline{c} \| \widetilde{W} \|_{2}^{2}$$

$$\tag{29}$$

for all  $W \in \mathcal{C}_0$  and  $\widetilde{W} = W_{\rm sh} - W$ .

*Proof.* By Assumption 3.1, the function  $g_{\Phi}$  is smooth and positive in (-1, 1) with

$$g_{\Phi}(\pm 1) = 0,$$
  $g'_{\Phi}(\pm 1) = 0,$   $g''_{\Phi}(\pm 1) = 1 - \Phi''(\pm 1),$ 

and hence we can choose  $\underline{c}$  and  $\overline{c}$  such that

$$\underline{c}(-1-w)^2 \leq g_{\Phi}(w) \leq \overline{c}(-1-w)^2 \qquad \text{for all} \quad -1 \leq w \leq 0,$$
 
$$\underline{c}(+1-w)^2 \leq g_{\Phi}(w) \leq \overline{c}(+1-w)^2 \qquad \text{for all} \quad 0 \leq w \leq +1.$$

This implies  $\underline{c}(\widetilde{W}(\varphi))^2 \leq g_{\Phi}(W(\varphi)) \leq \overline{c}(\widetilde{W}(\varphi))^2$  for all  $\varphi \in \mathbb{R}$ , and (29) follows thanks to (26).

Notice that the particular values of  $\underline{c}$  and  $\overline{c}$  depend on the choice of the pinning point (zero in  $\mathcal{C}_0$ ), and that there is no similar result for  $W \in \mathcal{C}$ . In fact, for any  $W \in \mathcal{C}$  we have  $\mathcal{L}_{\#}(W(\cdot + \bar{\varphi})) - \mathcal{L}_{\#}(W) = \mathcal{L}(W(\cdot + \bar{\varphi})) - \mathcal{L}(W) = 0$  but  $\|\widetilde{W}(\cdot + \bar{\varphi})\|_2 - \|\widetilde{W}\|_2 \to \infty$  as  $\bar{\varphi} \to \infty$ .

Combining Lemma 3.11 with Lemma 3.12 we finally find the desired bounds for  $\mathcal{L}$ .

**Corollary 3.13.** The sub-level sets of  $\mathcal{L}$  in  $\mathcal{C}_0$  are bounded in the following sense. For each  $c_1$  there exists  $c_2 > 0$  such that  $\mathcal{L}(W) \leq c_1$  implies  $\|\widetilde{W}\|_2 \leq c_2$ .

#### 3.5 Existence of minimisers

Now we can complete the existence proof for monotone supersonic fronts. To this end we study weakly convergent minimising sequences for  $\mathcal{L}$ , and exploit the following observations: The limit  $\bar{\gamma}$  of the kinetic energies of the minimising sequence and the kinetic energy  $\gamma_{\infty}$  of the weak limit satisfy  $\Delta \gamma = \bar{\gamma} - \gamma_{\infty} \geq 0$ . Consequently, the weak limit is a minimiser of  $\mathcal{L}$  if and only if the limiting potential energy difference is less than  $\Delta \gamma$ . To prove this, we first observe that the potential energy converges strongly on compact sets so that we only have to control the potential energy in the tails of the profile. Second, we show that the loss of potential energy in the tails is strictly less than  $\Delta \gamma$  provided the shock is supersonic.

**Theorem 3.14.**  $\mathcal{L}$  attains its minimum in  $\mathcal{C}$ . More precisely,  $\mathcal{L}$  is weakly lower semi-continuous on  $\widetilde{\mathcal{C}}_0$ , and each minimising sequence has a strongly convergent subsequence.

*Proof.* We first prove the minimisation in  $\mathcal{C}$  which consists of the following steps.

1. Let  $(W_n)_n \subset \mathcal{C}$  be a minimising sequence, i.e.  $\mathcal{L}(W_n) \to \inf \mathcal{L}|_{\mathcal{C}}$ . According to Corollary 3.10 we can suppose  $W_n \in \mathcal{C}_0$ , and Corollary 3.13 shows that the sequence  $(\widetilde{W}_n)_n \subset \widetilde{\mathcal{C}}_0$  with  $\widetilde{W}_n = W_{\rm sh} - W_n$  is bounded in  $\mathsf{L}^2$ . Hence we can extract a (not relabelled) subsequence such that

$$\widetilde{W}_n \to \widetilde{W}_\infty$$
 weakly in  $\mathsf{L}^2$ , and  $\gamma_n := \frac{1}{2} \parallel \widetilde{W}_n \parallel_2^2 \to \bar{\gamma} \geq \gamma_\infty := \frac{1}{2} \parallel \widetilde{W}_\infty \parallel_2$ 

for some weak limit  $\widetilde{W}_{\infty}$  corresponding to  $W_{\infty} = W_{\rm sh} - \widetilde{W}_{\infty}$ . Moreover, we have  $\widetilde{W}_{\infty} \in \widetilde{\mathcal{C}}_0$  and  $W_{\infty} \in \mathcal{C}_0$  as  $\widetilde{\mathcal{C}}_0$  is closed under weak convergence. Setting  $U_n := \widetilde{W}_n - \widetilde{W}_{\infty} = W_n - W_{\infty}$  we find

$$U_n \to 0$$
 weakly in  $L^2$ , and  $\frac{1}{2} \|U_n\|_2^2 \to \bar{\gamma} - \gamma_\infty$ , (30)

which implies

$$\mathcal{A}U_n \to 0$$
 and  $\mathcal{A}W_n \to \mathcal{A}W_\infty$  strongly and pointwise in  $\mathsf{L}^2([-M, M])$  (31)

for each  $M < \infty$ , see Lemma 3.3. With these notations we write

$$\mathcal{L}(W_n) - \mathcal{L}(W_\infty) = \int_{\mathbb{R}} \frac{1}{2} \Big( (W_\infty + U_n)^2 - W_\infty^2 \Big) - \Big( \Phi(\mathcal{A}W_\infty + \mathcal{A}U_n) - \Phi(\mathcal{A}W_\infty) \Big) \, \mathrm{d}\varphi$$
$$= I_{1, n} + I_{2, n} - I_{3, n},$$

where the  $I_{i,n}$ 's are given by

$$I_{1,n} := \frac{1}{2} \int_{\mathbb{R}} U_n^2 \, d\varphi,$$

$$I_{2,n} := \int_{\mathbb{R}} W_{\infty} U_n - \Phi'(\mathcal{A}W_{\infty}) \mathcal{A}U_n \, d\varphi = \int_{\mathbb{R}} \left( W_{\infty} - \mathcal{A}\Phi'(\mathcal{A}W_{\infty}) \right) U_n \, d\varphi,$$

$$I_{3,n} := \int_{\mathbb{R}} \Phi_{(\mathcal{A}W_{\infty})(\varphi)} \left( (\mathcal{A}U_n)(\varphi) \right) d\varphi,$$

and  $\Phi_{(\mathcal{A}W_{\infty})(\varphi)}(\cdot)$  are pointwise normalised potentials as in Remark 3.5.

2. Towards an estimate for  $I_{3,n}$ , we fix  $\varepsilon > 0$  sufficiently small, and  $M = M(\varepsilon)$  sufficiently large, such that

$$\sup_{|\varphi| > M} |W_{\rm sh}(\varphi) - (\mathcal{A}W_{\infty})(\varphi)| \le \frac{1}{2}\varepsilon. \tag{32}$$

The convergence (31) provides  $\mathcal{A}W_n(\pm M) \to \mathcal{A}W_\infty(\pm M)$ , hence

$$|(\mathcal{A}W_{\infty} - \mathcal{A}W_n)(-M)| + |(\mathcal{A}W_{\infty} - \mathcal{A}W_n)(M)| \le \frac{1}{2}\varepsilon$$

for all sufficiently large n, and since  $W_n$  is increasing we conclude that

$$\sup_{|\varphi| \ge M} |W_{\rm sh}(\varphi) - (\mathcal{A}W_n)(\varphi)| \le \varepsilon. \tag{33}$$

Combining (32) and (33) with Remark (3.5) we find

$$0 \le \Phi_{(\mathcal{A}W_{\infty})(\varphi)}((\mathcal{A}U_n)(\varphi)) \le \frac{\zeta_{\varepsilon}}{2}(\mathcal{A}U_n)(\varphi)^2$$
(34)

for  $|\varphi| \ge M$  and all sufficiently large n, where

$$\zeta_{\varepsilon} := \sup \Big\{ \Phi''(w) : w \in [-1, -1 + \varepsilon] \cup [1 - \varepsilon, 1] \Big\}.$$

With (34) and  $\|AU_n\|_2 \le \|U_n\|_2$  we now estimate

$$0 \leq I_{3,n} \leq \int_{|\varphi| \leq M} \Phi_{(\mathcal{A}W_{\infty})(\varphi)} ((\mathcal{A}U_n)\varphi) \, \mathrm{d}\varphi + \int_{|\varphi| \geq M} \Phi_{(\mathcal{A}W_{\infty})(\varphi)} ((\mathcal{A}U_n)\varphi) \, \mathrm{d}\varphi$$
$$\leq \frac{1}{2} \zeta_2 \int_{|\varphi| \leq M} (\mathcal{A}U_n)(\varphi)^2 \, \mathrm{d}\varphi + \frac{1}{2} \zeta_{\varepsilon} \int_{|\varphi| \geq M} (\mathcal{A}U_n)(\varphi)^2 \, \mathrm{d}\varphi$$
$$\leq \frac{1}{2} \zeta_2 \|(\mathcal{A}U_n)|_{[-M,M]} \|_2^2 + \frac{1}{2} \zeta_{\varepsilon} \|U_n\|_2^2,$$

and exploiting (31) and (30) we obtain  $\limsup_{n\to\infty} I_{3,n} \leq \zeta_{\varepsilon}(\bar{\gamma}-\gamma_{\infty})$ . Since  $\varepsilon$  was chosen arbitrarily, we derive

$$\lim_{n \to \infty} \sup I_{3, n} \le \zeta_0(\bar{\gamma} - \gamma_\infty),\tag{35}$$

where  $\zeta_0 = \max\{\Phi''(-1), \Phi''(1)\}\$  satisfies  $0 \le \zeta_0 < 1$  on account of Assumption 3.1.

3. Combining (35) with  $I_{1,n} \to \bar{\gamma} - \gamma_{\infty}$  and  $I_{2,n} \to 0$  we find

$$\lim_{n \to \infty} \mathcal{L}(W_n) \ge \mathcal{L}(W_\infty) + (1 - \zeta_0)(\bar{\gamma} - \gamma_\infty) \ge \mathcal{L}(W_\infty), \tag{36}$$

and since  $(W_n)_n$  is a minimising sequence, we also have

$$\mathcal{L}(W_{\infty}) \ge \lim_{n \to \infty} \mathcal{L}(W_n). \tag{37}$$

This shows  $\mathcal{L}(W_{\infty}) = \lim_{n \to \infty} \mathcal{L}(W_n)$ , so  $W_{\infty}$  is a minimiser of  $\mathcal{L}$  in  $\mathcal{C}$ .

Revising the proof so far yields the additional results: (i)  $\mathcal{L}$  is weakly lower semi-continuous on  $\widetilde{\mathcal{C}}_0$  as (36) holds even for non-minimising sequences. (ii) Concerning strongly convergent subsequences, (36) and (37) provide  $\bar{\gamma} = \gamma_{\infty}$  and hence  $\|\widetilde{W}_n\|_2 \to \|\widetilde{W}_{\infty}\|_2$ , which in turn implies that the weak convergence  $\widetilde{W}_n - \widetilde{W}_{\infty} \to 0$  is strong.

We have now finished the existence proof for action-minimising fronts with monotone profile. In particular, the second part of Theorem 1.1 follows by combining Lemma 2.2, Remark 2.3, Lemma 3.7 and Theorem 3.14.

We conclude with two remarks about the necessity of conditions (S) and (A).

(i) Suppose that  $\Phi$  satisfies (E) with strictly concave-convex  $\Phi'$ . Then the asymptotic states are subsonic with  $\Phi''(\pm 1) > 1$  and  $g_{\Phi}$  is negative in (-1, 1). Using (26) we show that (29) holds for negative constants  $\underline{c}, \overline{c} < 0$ , and since (27) still holds we conclude that  $\mathcal{L}$  is bounded from above but unbounded from below. In particular, action minimising fronts cannot exist and each minimising sequence diverges via  $\|\widetilde{W}\|_2 \to \infty$ . On the other hand, similar to the proof of Theorem 3.14 we can show that  $\mathcal{L}$  attains its maximum in  $\mathcal{C}$ . However, we cannot conclude that the maximiser solves the front equation, compare Remark 3.8, and numerical simulations indicate that the maximiser is not a front.

(ii) More generally, suppose (A) fails because there exist  $-1 < \hat{w} < +1$  with  $g_{\Phi}(\hat{w}) < 0$ , and define the sequence  $W_n \in \mathcal{C}$  with extending plateau at  $\hat{w}$  by  $W_n(\varphi) = \operatorname{sgn}\varphi$  for  $|\varphi| \geq n$  and  $W_n(\varphi) = \hat{w}$  for  $|\varphi| < n$ . Then (26) and (27) imply  $\mathcal{L}(W_n) \to -\infty$ , so action-minimising fronts cannot exist. Of course, this does not disprove the existence of local minimisers of  $\mathcal{L}$ , but the numerical simulation in §4.2 indicate that these do not exist.

## 4 Qualitative properties and numerical computation of fronts

### 4.1 Qualitative properties of fronts

In this section we discuss some aspects concerning the shape of front profiles W, which hold for any bounded and monotone solution  $W = W_{\rm sh} - \widetilde{W}$  to the front equation  $W = \mathcal{A}\Phi'(\mathcal{A}W)$ . Recall that such solutions belong to  $\mathbb{C}^2$  as noted in Remark 2.3.

Front profiles are actually strictly monotone for strictly convex  $\Phi$  for the following reason: First we note that there exists at least one  $\varphi_0$  such that  $W'(\varphi_0) > 0$ , and with  $W' \ge 0$  this implies  $(\mathcal{A}W')(\varphi) > 0$  for all  $\varphi \in (\varphi_0 - \frac{1}{2}, \varphi_0 + \frac{1}{2})$ . Moreover, the front equation implies

$$W' = \mathcal{A} \big[ \Phi''(\mathcal{A}W) \mathcal{A}W' \big],$$

and since  $\Phi'' > 0$  we infer that  $W'(\varphi) > 0$  for all  $\varphi \in (\varphi_0 - 1, \varphi_0 + 1)$ . Finally, by iterating this argument we find  $W'(\varphi) > 0$  for all  $\varphi \in \mathbb{R}$ .

We next study the convergence to the asymptotic states. Heuristically, the convergence to the constant states  $w = \pm 1$  is dictated by the linearisation in the asymptotic states, that is  $\widetilde{W} = \lambda_{\pm} \mathcal{A}^2 \widetilde{W}$ , with  $\lambda_{+} = \Phi''(1)$  and  $\lambda_{-} = \Phi''(-1)$  for right and left tails, respectively. Differentiating twice with respect to  $\varphi$  we find the linear advance-delay differential equation

$$\widetilde{W}'' = \lambda_{\pm} \Delta \widetilde{W},$$

with discrete Laplacian  $(\Delta \widetilde{W})(\varphi) = \widetilde{W}(\varphi+1) + \widetilde{W}(\varphi-1) - 2\widetilde{W}(\varphi)$ . The exponential ansatz  $\widetilde{W}(\varphi) = e^{-\tau \varphi}$  gives the characteristic equation

$$\tau^2 = 2\lambda_+(\cosh(\tau) - 1),$$

where decay corresponds to solutions  $\tau$  with negative real part and monotonicity requires  $\tau \in \mathbb{R}$ . Since supersonic speed implies  $0 < \lambda_{\pm} < 1$  in the normalised potential it is straightforward to see that the only nonnegative real roots of the characteristic equation are the double root  $\tau = 0$  and a simple root  $\tau_{\pm} > 0$ .

In conclusion, for monotone W the function W is expected to decay exponentially with rate  $\tau_+$  and  $\tau_-$  as  $\varphi \to +\infty$  and  $\varphi \to -\infty$ , respectively. We prove a weaker variant of this heuristic result for  $\varphi \to \infty$ , and mention that an analogous result characterizes the decay for  $\varphi \to -\infty$ .

**Lemma 4.1.** Let W be a monotone solution to (10). Then, for all  $\underline{\tau}$ ,  $\overline{\tau}$  with  $\underline{\tau} < \tau_+ < \overline{\tau}$  there exist positive constants  $\underline{c}$  and  $\overline{c}$  such that

$$\underline{c}\exp\left(-\overline{\tau}\varphi\right) \le \widetilde{W}(\varphi) \le \overline{c}\exp\left(-\underline{\tau}\varphi\right) \tag{38}$$

for all  $\varphi \geq 0$ .

The recently established existence of centre-stable manifolds for nonlinear advance-delay differential equations, [Geo08] Theorem 5.1, shows that nonlinear decay is precisely described by the linear decay except for the centre directions. Since  $\tau_+$  is an algebraically simple eigenvalue there is no secular growth and so Lemma 4.1 in fact implies that (38) holds for  $\overline{\tau} = \underline{\tau} = \tau_+$  and more precisely that there are constants  $a \neq 0$ ,  $\nu > 0$  such that

$$\widetilde{W}(\varphi) = a \exp(-\tau_{+}\varphi) + \mathcal{O}(\exp(-(\tau_{+} + \nu)\varphi).$$

Our point, however, is to obtain the decay rate using a direct approach with a rather simple proof. Not surprisingly, the same rates of decay describe the tails of small amplitude supersonic solitons in [FP99] Indeed, Lemma 4.1 requires monotonicity only in the tails and therefore also applies to all supersonic solitons with monotone tails, as these solve (10) after a suitable rescaling, compare [Her09].

*Proof.* We first show the existence of both exponentially decaying lower and upper bounds for  $\widetilde{W}$  and prove afterwards that  $\underline{\tau}$  and  $\overline{\tau}$  can be chosen arbitrary close to  $\tau_+$ .

1. By Taylor-expansions of  $\Phi$  around w=1 and due to  $(\widetilde{AW})(\varphi) \to 0$  as  $\varphi \to \infty$  we find for each  $0 < \delta < 1$  some  $\varphi_{\delta}$  such that

$$\lambda_{+}(1-\delta)(\mathcal{A}^{2}\widetilde{W})(\varphi) \leq \widetilde{W}(\varphi) \leq \lambda_{+}(1+\delta)(\mathcal{A}^{2}\widetilde{W})(\varphi) \quad \text{for all} \quad \varphi \geq \varphi_{\delta}. \tag{39}$$

Moreover, since  $\widetilde{W}$  is monotonically decreasing for  $\varphi \geq 0$  we have  $\|\widetilde{W}\|_2^2 \geq \int_0^{\varphi} \widetilde{W}(\tilde{\varphi})^2 d\tilde{\varphi} \geq \varphi \widetilde{W}(\varphi)^2$ , and hence

$$0 \le \widetilde{W}(\varphi) \le \|\widetilde{W}\|_2 \varphi^{-1/2}. \tag{40}$$

2. An important building block for the upper bound is the implication

$$U(\varphi) \le C\varphi^{-1/2} \quad \forall \, \varphi > 0 \qquad \Longrightarrow \qquad (\mathcal{A}^2 U)(\varphi + 1) \le C\varphi^{-1/2} \quad \forall \, \varphi > 0, \tag{41}$$

which follows from a direct computation of  $\mathcal{A}^2[\varphi^{-1/2}]$ . For fixed  $\delta$  and  $\varphi \geq \varphi_{\delta}$  we combine the previous results as follows: (40) and (41) imply  $(\mathcal{A}^2\widetilde{W})(\varphi+1) \leq \|\widetilde{W}\|_2 \varphi^{-1/2}$  and with (39) we find

$$0 \le \widetilde{W}(\varphi + 1) \le \lambda_{+}(1 + \delta) \|\widetilde{W}\|_{2} \varphi^{-1/2}.$$

Using (41) for  $U(\varphi) = \widetilde{W}(\varphi + 1)$  we obtain  $(A^2\widetilde{W})(\varphi + 2) \le \lambda_+(1 + \delta) \|\widetilde{W}\|_2 \varphi^{-1/2}$ , and (39) yields

$$0 \le \widetilde{W}(\varphi + 2) \le \lambda_+^2 (1 + \delta)^2 \|\widetilde{W}\|_2 \varphi^{-1/2}.$$

Iterating these arguments gives

$$0 \le \widetilde{W}(\varphi + n) \le \lambda_{+}^{n} (1 + \delta)^{n} \| \widetilde{W} \|_{2} \varphi^{-1/2} \quad \forall \varphi \ge \varphi_{\delta} \ \forall \ n \in \mathbb{N},$$

and since  $\delta$  was arbitrary we have established the upper estimate in (38) for some  $\underline{\tau}$  with  $\underline{\tau} > -\ln \lambda_+ > 0$  and some sufficiently large  $\overline{c}$ .

3. Concerning a lower bound, the monotonicity of  $\widetilde{W}$  for  $\varphi > 0$  implies  $(\widetilde{AW})(\varphi + \frac{1}{4}) \ge \frac{1}{4}\widetilde{W}(\varphi)$ , and therefore  $(A^2\widetilde{W})(\varphi + \frac{1}{2}) \ge \frac{1}{16}\widetilde{W}(\varphi)$ . Combination with (39) gives

$$\widetilde{W}(\varphi + \frac{1}{2}) \ge \frac{1}{16}(\lambda_{+}(1-\delta))\widetilde{W}(\varphi) \quad \forall \ \varphi \ge \varphi_{\delta},$$

and by iteration we show the existence of an exponentially decaying lower bound.

4. Using the previous step we now assume that (38) holds for some constants  $\underline{c}$ ,  $\overline{c}$ , and some rates  $0 < \underline{\tau} < \tau_+ < \overline{\tau}$ , and show that these rates can be improved. In relation to the above characteristic equation we define the function  $\varrho(\tau) := 2\tau^{-2}(\cosh(\tau) - 1)$  and observe that  $\mathcal{A}^2[e^{-\tau\varphi}] = \rho(\tau)e^{-\tau\varphi}$ . Hence, for all  $\tau > 0$  and  $\varphi_* > 0$  we have

$$U(\varphi) \leq C \exp\left(-\tau \varphi\right) \quad \forall \ \varphi > \varphi_* \qquad \Longrightarrow \qquad \left(\mathcal{A}^2 U\right)(\varphi) \leq C \varrho(\tau) \exp\left(-\tau \varphi\right) \quad \forall \ \varphi > \varphi_* + 1. \ \ (42)$$

Due to (39) and using an iteration argument similar to the above one we arrive at

$$\widetilde{W}(\varphi) \le C(\lambda_{+}(1+\delta)\varrho(\tau))^{n} \exp(-\tau\varphi) \qquad \forall \ \varphi \ge \varphi_{\delta} + n \ \forall \ n \in \mathbb{N}, \tag{43}$$

and since  $\widetilde{W}$  is decreasing this implies

$$\widetilde{W}(\varphi_{\delta} + \varphi) \leq \widetilde{C}(\lambda_{+}(1+\delta)\varrho(\tau))^{\varphi} \exp(-\tau\varphi)$$

for all  $\delta > 0$ ,  $\tau > 0$ ,  $\varphi \ge 0$  and some constant  $\tilde{C}$ . Therefore we can improve the assumed decay rate  $\underline{\tau}$  provided that  $\lambda_{+}\varrho(\underline{\tau}) < 1$ , that means  $\underline{\tau} < \tau_{+}$ . More precisely, choosing  $\delta$  sufficiently small and adapting the constant  $\overline{c}$  we derive from (43) that the upper estimate in (38) also holds for the new rate

$$\underline{\tau} = \underline{\tau} - \ln\left(\frac{1}{2}(\lambda_{+}\varrho(\underline{\tau}) + 1)\right) > \underline{\tau}.$$

Since the iteration of the map  $\underline{\tau} \mapsto \underline{\tau}$  yields a strictly increasing sequence that converges to  $\tau_+$ , we conclude that  $\underline{\tau}$  can be chosen arbitrarily close to  $\tau_+$ . Finally, reversing the inequality signs on both sides of the implication (42) we can show that  $\overline{\tau}$  can also be chosen arbitrarily close to  $\tau_+$ .

### 4.2 Numerical computation of fronts

In view of Theorem 3.14 it seems natural to approximate fronts by using some discrete counterpart of the gradient flow of  $\mathcal{L}$ , as for instance the explicit Euler scheme (23).

A corresponding numerical scheme on a finite interval is readily derived and implemented, but from the rigorous point of view the account of such a scheme is limited: (i) There is no convergence proof. (ii) Due to the lack of uniqueness results it is not clear whether or not our existence result covers all fixed points of the scheme.

Nevertheless, such schemes work very well numerically and provide moreover some intuitive understanding for why energy conservation, supersonic front speed, and area condition are necessary for the existence of action minimising fronts.

We start with functions  $\Phi'$  that have exactly one turning point. A positive example with admissible potential  $\Phi$ , initial profile  $W_0 = W_{\rm sh}$ , and  $\lambda = 1$  is plotted in Figure 5. After a small number of iterations the profile W becomes stationary and satisfies the front equation up to high order; the same qualitative behaviour can be observed for other  $0 \le \lambda \le 1$  and other initial data  $W_0 \in \mathcal{C}$ .

In Figure 6 we plot the result for the same scheme applied to a potential that does not satisfy the energy conservation. Here the profiles do not converges to a front solution, but instead form a travelling wave for the iteration: After some initial iterations we find a stationary profile that is shifted in each step. Recall that in this case the action functional  $\mathcal{L}$  is not invariant under shifts, and thus the profiles successively decrease their action by converging to the asymptotic state with higher potential energy. More precisely, assuming  $\mathcal{T}(W) = W(\cdot + \bar{\varphi})$  and exploiting (25) we find  $0 \leq \triangle \mathcal{L} = \mathcal{L}(W) - \mathcal{L}(\mathcal{T}[W]) = \bar{\varphi}(\Phi(1) - \Phi(-1))$ , and hence  $\operatorname{sgn}(\bar{\varphi}) = \operatorname{sgn}(\Phi(1) - \Phi(1)) < 1$ .

In order to understand the role of supersonic fronts we next consider potentials that conserve the energy with concave-convex  $\Phi'$ . Such potentials are prototypical for subsonic conservative shocks and have unbounded  $\mathcal{L}$  as discussed at the end of §3. Figure 7 illustrates that the iteration scheme generates a plateau with increasing length and two counterpropagating travelling waves that connect the plateau to the asymptotic states. The height of the plateau is the unique solution to  $\bar{w} = \Phi'(\bar{w})$  with  $-1 < \bar{w} < 1$ , and as above we conclude that the decrease in  $\mathcal{L}$  is given by  $\Delta \mathcal{L} = \bar{\varphi}_1(\Phi(\bar{w}) - \Phi(-1)) + \bar{\varphi}_2(\Phi(1) - \Phi(\bar{w}))$ , where  $\bar{\varphi}_1 > 0$  and  $\bar{\varphi}_2 < 0$  are the pase shifts for the travelling waves.

Finally, we study two potentials that both have three turning points in the distance jump of supersonic conservative shock data. The numerical simulations in Figure 8 and Figure 9 indicate that the signed area condition is truly necessary for the existence of action minimising fronts. If this condition fails the profiles create again an extending plateau and two counter-propagating travelling waves, where the plateau height  $\bar{w}$  satisfies  $\Phi'(\bar{w}) = \bar{w}$  and  $\Phi''(w) < 1$ .

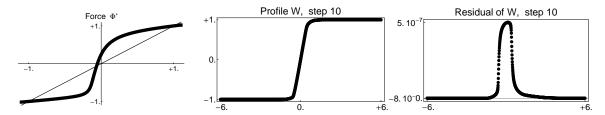


Figure 5: Example 1 with  $\Phi$  as in Assumption 3.1: The profiles converge to a front.

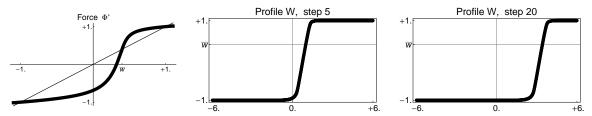


Figure 6: Example 2 with  $\Phi(1) \neq \Phi(-1)$ : The profiles minimise the action through subsequent shifts and converge to a constant.

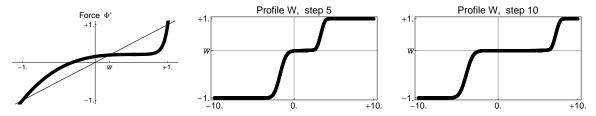


Figure 7: Example 3 with  $\Phi''(\pm 1) > 1$ : The profiles converge to a constant via an extending plateau.

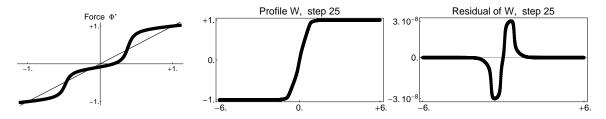


Figure 8: Example 4 with area condition: The profiles converge to a front.

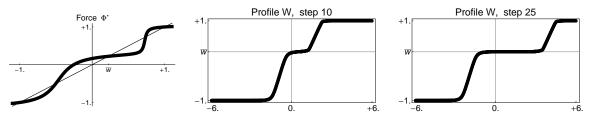


Figure 9: Example 5 without area condition: The profiles generate an extending plateau.

## Acknowlegdements

This work has been supported in part by the DFG Priority Program 1095 "Analysis, Modeling and Simulation of Multiscale Problems" (M.H., J.R.), and the NDNS+ cluster of the Netherlands Organisation for Scientific Research NWO (J.R.). We thank the reviewers for their insightful comments and for pointing us to additional references.

### References

- [AP07] S. Aubry and L. Proville, *Pressure Fronts in 1D Nonlinear Lattices*, to appear in proceedings of EQUADIFF-07, 2007.
- [Daf00] C.M. Dafermos, *Hyperbolic conservation laws in continuum physics*, Grundlehren d. mathem. Wissenschaften, vol. 325, Springer, Berlin, 2000.
- [DHM06] W. Dreyer, M. Herrmann, and A. Mielke, *Micro-macro transition for the atomic chain via Whitham's modulation equation*, Nonlinearity **19** (2006), no. 2, 471–500.
- [FP99] G. Friesecke and R.L. Pego, Solitary waves on FPU lattices. I. Qualitative properties, renormalization and continuum limit, Nonlinearity 12 (1999), no. 6, 1601–1627.
- [FPU55] E. Fermi, J. Pasta, and S. Ulam, *Studies on nonlinear problems*, Los Alamos Scientific Laboraty Report LA–1940, 1955, reprinted in: D.C. Mattis (editor), The many body problem. World Scientific, 1993.
- [FV99] A.-M. Filip and S. Venakides, Existence and modulation of traveling waves in particle chains, Comm. Pure Appl. Math. **51** (1999), no. 6, 693–735.
- [FW94] G. Friesecke and J.A.D. Wattis, Existence theorem for solitary waves on lattices, Comm. Math. Phys. **161** (1994), no. 2, 391–418.
- [Geo08] M. Georgi, Homoclinic solutions and Hopf bifurcations in functional differential equations of mixed type, to appear in Proc. R. Soc. Edingburgh, Section A, 2008.
- [Her05] M. Herrmann, Ein Mikro-Makro-Übergang für die nichtlineare atomare Kette mit Temperatur, Phd thesis, Humboldt-Universität zu Berlin, 2005.
- [Her09] \_\_\_\_\_, Unimodal wave trains and solitons in convex FPU chains, arXiv:0901.3736, 2009.
- [HR08] M. Herrmann and J. Rademacher, Riemann solvers and undercompressive shocks in FPU chains, submitted, 2008.
- [IJ05] G. Iooss and G. James, Localized waves in nonlinear oscillator chains, Chaos 15 (2005), 015113.
- [Ioo00] G. Iooss, Travelling waves in the Fermi-Pasta-Ulam lattice, Nonlinearity 13 (2000), 849–866.
- [LeF02] P.G. LeFloch, *Hyperbolic systems of conservation laws*, Lectures in Mathematics: ETH Zürich, Birkhäuser, Basel, 2002.
- [Pan05] A. Pankov, Traveling Waves and Periodic Oscillations in Fermi-Pasta-Ulam lattices, Imperial College Press, London, 2005.
- [PP00] A. Pankov and K. Pflüger, Traveling Waves in Lattice Dynamical Systems, Math. Meth. Appl. Sci. 23 (2000), 1223–1235.
- [SCC05] L. Slepyan, A. Cherkaev, and E. Cherkaev, Transition waves in bistable structures. II. Analytical solution: wave speed and energy dissipation, J. Mech. Phys. Solids **53** (2005), 407–436.
- [Ser07] D. Serre, Discrete shock profiles: Existence and stability, Hyperbolic Systems of Balance Laws, Lecture Notes in Mathematics, vol. 1991, Springer, 2007, pp. 79–158.
- [Smo94] J. Smoller, *Shock waves and reaction-diffusion equations*, 2. ed., Grundlehren d. mathem. Wissenschaften, vol. 258, Springer, 1994.
- [SW97] D. Smets and M. Willem, Solitary waves with prescribed speed on infinite lattices, J. Funct. Anal. 149 (1997), 266–275.

- [SZ07] H. Schwetlick and J. Zimmer, Solitary waves for nonconvex FPU lattices, J. Nonlinear Sci. 17 (2007), no. 1, 1–12.
- [SZ08] \_\_\_\_\_\_, Existence of dynamic phase transitions in a one-dimensional lattice model with piecewise quadratic interaction potential, submitted, 2008.
- [TV05] L. Truskinovsky and A. Vainchtein, *Kinetics of martensitic phase transitions: lattice model*, SIAM J. Appl. Math. **66** (2005), 533–553.